A New Understanding of Chemical Agent Release

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Abstract

The evolution of thickened chemical agent released at supersonic velocities, due to a missile defense intercept or a properly functioning warhead, has been misunderstood. Current and historical experimental and modeling efforts have attributed agent breakup to a variety of droplet breakup mechanisms. According to this model, drops of agent fragment into subsequent generations of smaller drops until a stable drop size is reached. Recent experimental data conducted in a supersonic wind tunnel show that agent breakup is not driven by any droplet breakup mechanism. The breakup of agent is instead governed by viscoelastic behavior and aerodynamic history effects. This viscoelastic breakup mechanism results in the formation of threads and sheets of liquid, instead of drops. The evolution and final state of agent released has broad implications not only for aerobreakup models, but also for all atmospheric dispersion models.

Problem Definition

The problem of lethal ground effects centers around the fallout of chemical agent, resulting from either a successful ballistic missile intercept or the proper functioning of an incoming chemical warhead. The lethal effect of agent fallout is influenced by two factors, the first is the individual sizes of agent masses which are correlated with lethal dose levels [1], the second is the areal density of ground deposition produced by fallout. The physical processes that dispersed agent experiences after release are complex, often interconnected, and wrought with attendant uncertainties. The presence of uncertainty in complex problems, which obviates deterministic approaches, requires one to consider the concept of risk and risk assessment. Implementing a good methodical approach to measure risk aids a whole range of decision making issues including avoidance of heavy ground casualties, optimizing defensive deployment and being adequately prepared for mitigation or remedial actions following a hazardous release of agent.

Supersonic Wind Tunnel ALPHA

The liquid breakup experiments were carried out on a transient, supersonic wind tunnel (ALPHA) constructed especially for this purpose. The ALPHA facility is illustrated in Figure 1 and the actual arrangement is shown in Figure 2. ALPHA was designed to test the stability of large liquid masses over long observation time scales (in the hundreds of milliseconds). The flexible design of the ALPHA facility also permitted the generation of "tailored" flow conditions that could be used to explore aerodynamic history effects. ALPHA is capable of reaching operating pressures ranging from 3 bar down to 5.e-4 bar, and with the acquisition of a better vacuum pump we believe that pressures of 1.e-5 bar can be reached. Exchanging flow nozzles will allow ALPHA to achieve flow Mach numbers ranging from $1 < M < 5$ which more than cover the range of supersonic flow conditions of interest. Significant aerodynamic effects experienced by agent begin at approximately the 70 km (7.e-5 bar pressure) level. The ambient air density gradually increases below this level, increasing the amount of aerodynamic drag experienced by the falling agent mass. As shown in Figure 3, the combination of operating pressures and supersonic velocities that ALPHA can achieve more than cover the relevant range of exo and endo-atmospheric conditions needed. Figure 3 contrasts the native capability of ALPHA compared to shock tubes, which are widely used in diagnosing liquid breakup. The difference in capability is obvious. No other liquid breakup facility of this type exists anywhere in the research and development community.

Defining the aerodynamic stability limits for agent masses requires a set of parameters that consider the competing aerodynamic force exerted by the supersonic flow field versus the internal restoring force of the drop.

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Abstract

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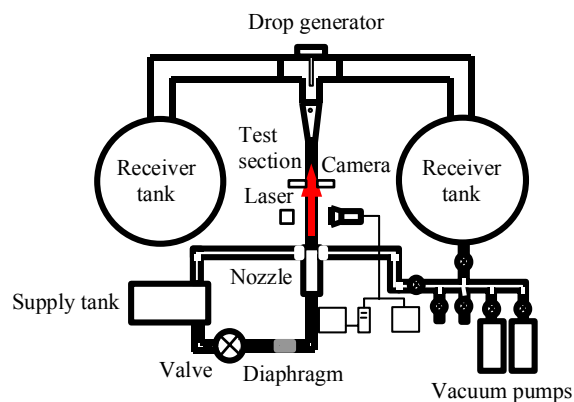| Classification of Abstract	Limitation of Abstract
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Figure 1. Schematic of the transient, supersonic wind tunnel ALPHA
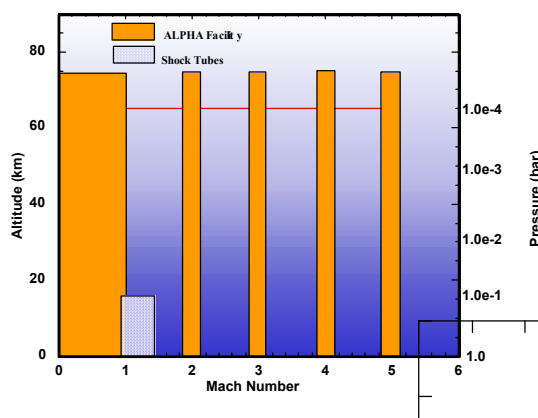

Figure 2. Picture of ALPHA facility

Figure 3. Diagram of the operating range of ALPHA and Shock Tubes

One such dimensionless parameter is the Weber number, shown as:

$$We = \frac{\rho v^2 D}{\sigma} \qquad (1)$$

Where ρ is the air density, v is the flow velocity, D is the scale size of interest, and σ is the surface tension of the drop. The Weber number shows the ratio between the aerodynamic pressure force, which distorts the mass, and the surface tension force, which acts to restore the minimum energy configuration. The purpose of the initial ALPHA experiments was to examine the breakup mechanism of liquid released at various altitudes and speeds. The variable parameters in the experiment are the pressures at the supply and receiving tanks, which regulate the velocity and density of the air flow in the test section. Exo and Endo-atmospheric release conditions at supersonic velocities can result in a wide range of Weber numbers from $1 < We < 10^5$. Table 1 shows the range of Weber numbers that can be accessed by ALPHA.

M	Pressure ratio	We Pr = 1Pa	We Ps = 1bar	We Ps = 3bar
1	1.9	0.3	10000	30000
2	7.8	1.0	10000	30000
3	36.7	2.0	5000	15000
4	151	4.0	2000	6000
5	529	6.0	1000	3000

Drop diameter = 5mm, Surface tension = 0.0273 N/m

Pr: Pressure in the Receiver tanks
Ps: Pressure in the Supply tank

Table 1. Operating range of ALPHA in terms of Weber number

Experimental Results

The experiments were carried out using Mach 3 flow conditions at air densities ranging from Sea Level, Normal-Pressure-Temperature (NPT), to 70 km altitude. The liquid used for this series of tests was TBP thickened with a few percent of PSBMA polymer. The objectives of this set of experiments was to identify the critical mechanism(s) dominating agent breakup and examine the post-breakup geometry and size of liquid masses.

Two cameras were used on ALPHA for this test series. One camera was located nearer the accelerating nozzle while the other was located downstream of the flow. Each camera captured a different stage in the liquid breakup process. The downstream camera captured images of the resultant liquid geometries and masses resulting from the observed breakup process. Many test runs were conducted to observe the reproducibility of the breakup mechanisms. No variation in the nature of the breakup mechanism was observed over various gas densities and liquid mass sizes and geometries.

Figure 4 shows the results of breakup of viscoelastic liquid at 32 and 34 milliseconds after initial flow impingement on the liquid mass.
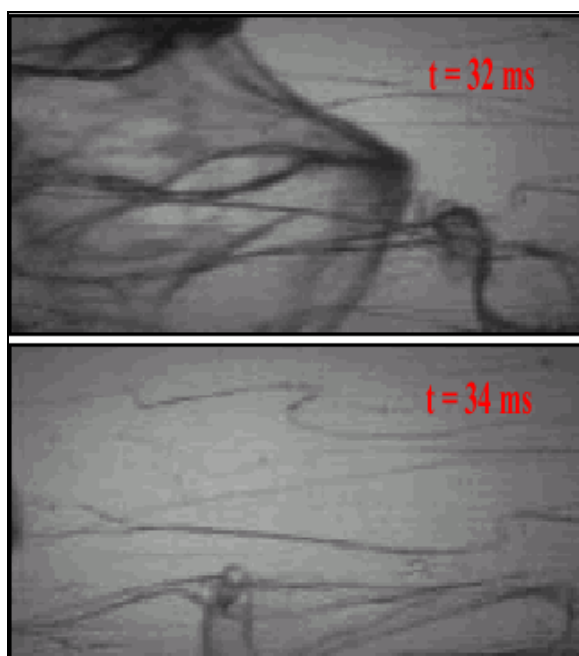
Figure 4. Liquid breakup using 3.8%PSBMA (M.W. 2,270,000)+TBP, d=15mm, We =3,500.

The viscoelastic breakup observed is characterized by the formation of threads and sheets of liquid due to aerodynamic shear forces that "drain" the initial liquid mass. The viscoelastic breakup mechanism does not appear to change significantly as a function of gas density and velocity. Figure 5 shows a frame from a Mach 3 flow with background pressure of ~0.1 mbar. The basic character of the breakup, involving the stretching and tearing under shear, of the liquid does not change as a function of gas density (altitude). However, the complexity of the thread network qualitatively increases as the Weber number increases. History effects become important due to the nature of the viscoelastic breakup.

The resistance of the fluid to fragmentation and gas interpenetration can be attributed to the total fraction of polymer added as well as the polymer molecular weight (M.W.).

Figure 5. Liquid breakup using 3.8%PSBMA (M.W. 2,270,000)+TBP, d=1.9 mm, We =30.

Variations in the fraction of added polymer material as well as variations in polymer molecular weight were tested under different flow conditions. Higher molecular weight polymer increases the resistance of the liquid to aerodynamic forces. As the total amount of added polymer is increased to representative levels, the viscoelastic breakup behavior dominates and any resemblance of the breakup to classic Newtonian droplet breakup disappears.

Conclusion

Liquid breakup tests conducted in representative velocity and gas density conditions show a viscoelastic breakup mechanism that is completely unlike classic Newtonian droplet breakup mechanisms [2] (Rayleigh-Taylor, Shear stripping, Bag, Oscillatory). This behavior has been observed in Mach 3 flow over a range of altitude representative conditions (0 < H < 70 km). The viscoelastic breakup behavior has been shown to be reproducible over many test runs.

The implications of these experimental results are significant.

• There is no basis for using droplet breakup mechanisms to describe aerobreakup, there are no drops.

• In the absence of a post-breakup thread particulation mechanism, which could fragment threads into drops, all current atmospheric dispersion codes would have to be modified to model the dispersion of threads and filaments.

Clearly further work is needed to understand the initial viscoelastic breakup as well as any post-breakup evolution of the thread and filament networks. Understanding both the viscoelastic material effects as well as the role of aerodynamic history is vital to solving the aerobreakup problem.

References

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2. Kolev, N.I., "Fragmentation and Coalescence Dynamics in Multiphase Flows", Experimental, *Thermal and Fluid Science*, **6**, No. 3, pp. 211-251, 1993.

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